



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:27 AM UTC

PDB ID : 2DHC / pdb_00002dhc
Title : CRYSTALLOGRAPHIC ANALYSIS OF THE CATALYTIC MECHANISM
OF HALOALKANE DEHALOGENASE
Authors : Verschueren, K.H.G.; Dijkstra, B.W.
Deposited on : 1993-09-08
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

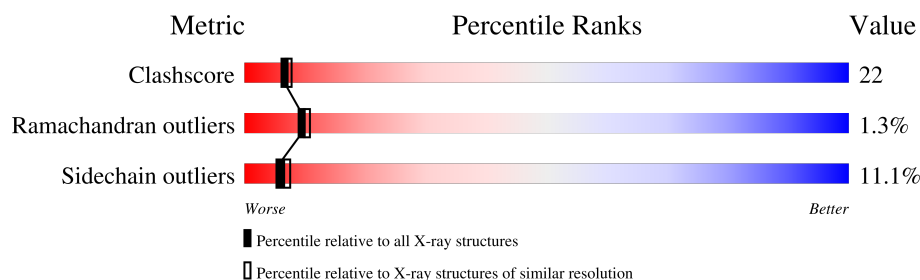
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DCE	A	600	-	-	X	-

2 Entry composition [i](#)

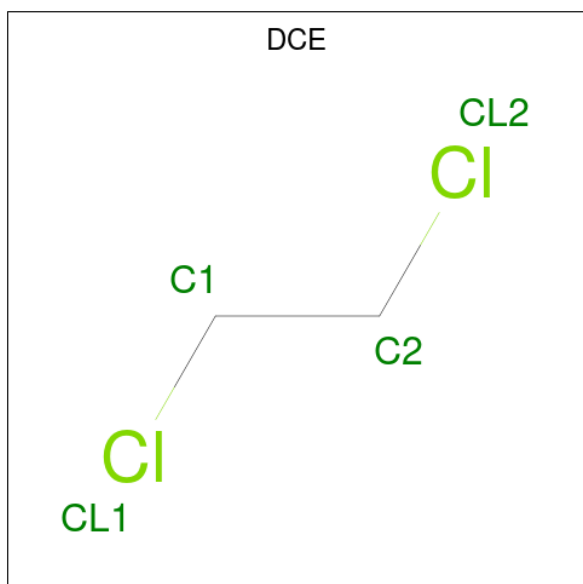
There are 3 unique types of molecules in this entry. The entry contains 2605 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HALOALKANE DEHALOGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2479	1596	406	462	15	0	0	0

- Molecule 2 is 1,2-DICHLOROETHANE (CCD ID: DCE) (formula: C₂H₄Cl₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	Cl		
2	A	1	4	2	2	0	0

- Molecule 3 is water.

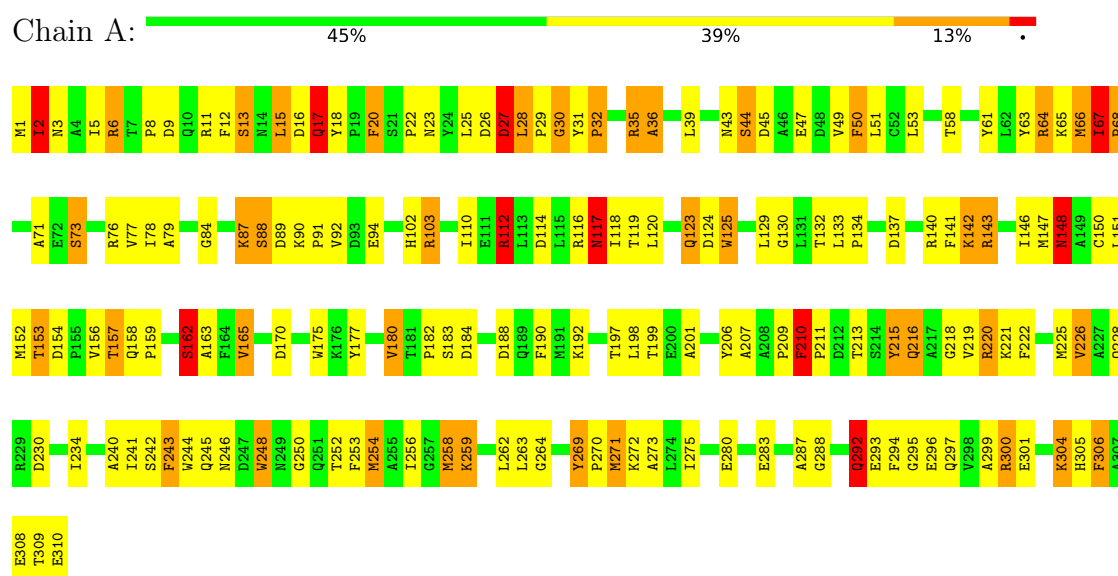
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	122	122	122	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: HALOALKANE DEHALOGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.90Å 72.80Å 41.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2605	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DCE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.10	2/2552 (0.1%)	2.26	132/3470 (3.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	GLU	N-CA	7.12	1.56	1.46
1	A	248	TRP	NE1-CE2	-5.58	1.31	1.37

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	PHE	CA-C-N	10.77	131.89	119.94
1	A	294	PHE	C-N-CA	10.77	131.89	119.94
1	A	228	GLN	CA-C-N	9.23	135.75	121.99
1	A	228	GLN	C-N-CA	9.23	135.75	121.99
1	A	3	ASN	CA-CB-CG	8.59	121.19	112.60
1	A	188	ASP	CA-C-N	8.38	131.84	120.44
1	A	188	ASP	C-N-CA	8.38	131.84	120.44
1	A	219	VAL	N-CA-C	-8.28	102.75	110.53
1	A	114	ASP	CA-CB-CG	8.20	120.80	112.60
1	A	199	THR	CA-CB-OG1	-8.08	97.47	109.60
1	A	295	GLY	N-CA-C	7.99	121.77	112.50
1	A	137	ASP	CA-CB-CG	-7.78	104.82	112.60
1	A	210	PHE	CA-C-N	7.66	127.55	119.05
1	A	210	PHE	C-N-CA	7.66	127.55	119.05
1	A	280	GLU	O-C-N	-7.61	112.57	121.32
1	A	87	LYS	N-CA-CB	7.47	122.20	110.46
1	A	22	PRO	CB-CA-C	-7.43	98.44	110.25
1	A	219	VAL	CA-C-N	7.30	129.94	120.44
1	A	219	VAL	C-N-CA	7.30	129.94	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	PRO	CA-C-O	-7.27	113.04	121.98
1	A	177	TYR	CB-CA-C	7.24	122.25	110.88
1	A	27	ASP	N-CA-CB	-7.20	101.11	111.54
1	A	220	ARG	N-CA-C	7.04	118.60	111.07
1	A	218	GLY	O-C-N	6.96	131.74	122.70
1	A	50	PHE	CA-CB-CG	-6.94	106.86	113.80
1	A	230	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	273	ALA	N-CA-C	6.92	121.47	112.89
1	A	148	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	A	117	ASN	CB-CA-C	6.90	121.53	111.73
1	A	271	MET	N-CA-C	-6.89	103.70	111.14
1	A	294	PHE	N-CA-C	-6.82	101.55	111.30
1	A	20	PHE	O-C-N	6.77	131.01	123.16
1	A	118	ILE	N-CA-C	6.65	117.66	108.89
1	A	254	MET	CB-CA-C	6.64	122.06	109.37
1	A	234	ILE	N-CA-CB	6.63	119.06	110.57
1	A	30	GLY	N-CA-C	-6.58	106.86	114.69
1	A	116	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	A	240	ALA	O-C-N	-6.55	114.68	122.15
1	A	118	ILE	O-C-N	6.47	129.99	122.81
1	A	71	ALA	O-C-N	-6.41	115.47	122.07
1	A	102	HIS	CA-CB-CG	6.40	120.20	113.80
1	A	163	ALA	N-CA-C	6.40	119.07	111.33
1	A	114	ASP	CA-C-O	-6.38	114.16	122.45
1	A	182	PRO	N-CA-CB	6.35	108.96	103.31
1	A	92	VAL	N-CA-C	6.29	119.87	111.44
1	A	201	ALA	N-CA-CB	6.23	119.38	110.16
1	A	32	PRO	N-CA-CB	6.20	108.82	103.36
1	A	3	ASN	O-C-N	-6.18	115.32	122.93
1	A	305	HIS	CA-CB-CG	6.17	119.97	113.80
1	A	18	TYR	O-C-N	-6.17	115.81	121.42
1	A	264	GLY	CA-C-N	6.16	127.54	119.84
1	A	264	GLY	C-N-CA	6.16	127.54	119.84
1	A	17	GLN	CB-CA-C	6.04	121.06	111.51
1	A	209	PRO	CB-CA-C	-6.03	102.33	111.44
1	A	241	ILE	CA-C-O	6.01	127.66	121.41
1	A	27	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	243	PHE	CA-CB-CG	-5.97	107.83	113.80
1	A	150	CYS	CB-CA-C	-5.96	101.57	113.80
1	A	159	PRO	O-C-N	-5.96	114.53	122.22
1	A	68	PRO	CB-CA-C	-5.94	103.44	112.11
1	A	103	ARG	NE-CZ-NH1	-5.93	115.57	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ASN	N-CA-CB	5.92	121.07	112.13
1	A	16	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	76	ARG	O-C-N	-5.90	116.60	123.27
1	A	162	SER	N-CA-C	-5.89	105.35	113.18
1	A	29	PRO	N-CA-CB	5.87	107.17	103.23
1	A	28	LEU	CB-CA-C	5.80	119.94	109.61
1	A	66	MET	CA-C-N	5.80	126.00	120.43
1	A	66	MET	C-N-CA	5.80	126.00	120.43
1	A	180	VAL	N-CA-C	5.77	120.92	113.07
1	A	150	CYS	N-CA-CB	5.76	118.69	110.51
1	A	102	HIS	N-CA-C	-5.75	106.42	113.50
1	A	47	GLU	CA-C-N	5.74	129.70	121.50
1	A	47	GLU	C-N-CA	5.74	129.70	121.50
1	A	201	ALA	CB-CA-C	5.68	120.51	110.85
1	A	20	PHE	CA-C-O	-5.67	114.40	120.92
1	A	184	ASP	CA-C-N	5.65	130.40	121.99
1	A	184	ASP	C-N-CA	5.65	130.40	121.99
1	A	143	ARG	CD-NE-CZ	5.65	132.30	124.40
1	A	244	TRP	CD2-CE2-CZ2	-5.57	116.83	122.40
1	A	78	ILE	N-CA-C	-5.53	100.66	109.17
1	A	216	GLN	N-CA-C	5.53	119.72	112.92
1	A	67	ILE	O-C-N	5.52	123.95	120.42
1	A	140	ARG	CB-CA-C	-5.52	100.87	110.09
1	A	226	VAL	CA-C-N	5.50	128.11	120.63
1	A	226	VAL	C-N-CA	5.50	128.11	120.63
1	A	71	ALA	CA-C-O	5.49	126.59	120.82
1	A	199	THR	N-CA-C	-5.47	102.37	110.46
1	A	198	LEU	CA-C-O	-5.43	112.75	120.51
1	A	66	MET	CA-C-O	5.42	126.61	120.00
1	A	165	VAL	O-C-N	5.42	129.24	121.82
1	A	36	ALA	CA-C-O	-5.40	115.06	121.16
1	A	65	LYS	N-CA-C	-5.38	106.72	113.72
1	A	242	SER	CA-C-N	5.38	127.76	120.44
1	A	242	SER	C-N-CA	5.38	127.76	120.44
1	A	263	LEU	CA-C-O	-5.37	112.83	120.51
1	A	35	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	A	306	PHE	N-CA-C	5.35	117.80	111.33
1	A	140	ARG	CA-C-O	-5.34	113.10	119.35
1	A	13	SER	CB-CA-C	-5.34	101.92	110.79
1	A	27	ASP	CB-CA-C	-5.30	102.91	111.18
1	A	6	ARG	NE-CZ-NH2	5.29	123.97	119.20
1	A	2	ILE	CB-CA-C	-5.29	104.55	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	TYR	CA-C-O	5.29	125.48	119.18
1	A	269	TYR	CA-CB-CG	-5.29	104.38	113.90
1	A	112	ARG	CB-CA-C	5.28	119.50	110.74
1	A	256	ILE	N-CA-CB	5.25	118.66	111.41
1	A	219	VAL	N-CA-CB	5.23	117.27	110.57
1	A	264	GLY	O-C-N	5.22	126.99	121.77
1	A	141	PHE	CA-C-O	-5.22	115.18	120.71
1	A	63	TYR	N-CA-CB	-5.20	101.68	110.41
1	A	141	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	76	ARG	CA-C-N	-5.17	116.78	123.19
1	A	76	ARG	C-N-CA	-5.17	116.78	123.19
1	A	125	TRP	CA-C-O	5.17	125.74	119.49
1	A	259	LYS	CA-C-N	-5.15	114.93	122.19
1	A	259	LYS	C-N-CA	-5.15	114.93	122.19
1	A	300	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	A	245	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	A	209	PRO	N-CA-CB	5.11	108.21	103.41
1	A	246	ASN	N-CA-C	5.10	119.50	113.12
1	A	77	VAL	O-C-N	-5.08	117.84	123.18
1	A	35	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	A	170	ASP	CA-CB-CG	-5.07	107.53	112.60
1	A	199	THR	CA-C-O	-5.07	115.45	121.89
1	A	26	ASP	CA-C-O	5.05	125.64	119.78
1	A	73	SER	CA-C-O	5.05	124.91	119.15
1	A	228	GLN	CA-C-O	-5.02	115.35	121.58
1	A	23	ASN	O-C-N	-5.01	116.67	123.19
1	A	49	VAL	CB-CA-C	-5.01	103.22	110.63
1	A	292	GLN	N-CA-CB	5.01	118.95	110.49
1	A	65	LYS	CG-CD-CE	5.01	122.81	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2479	0	2379	105	0
2	A	4	0	0	3	0
3	A	122	0	0	13	0
All	All	2605	0	2379	105	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:THR:HG21	1:A:158:GLN:HB2	1.33	1.10
1:A:292:GLN:HE21	1:A:292:GLN:H	1.04	0.99
1:A:133:LEU:HB2	1:A:134:PRO:HD3	1.59	0.84
1:A:304:LYS:O	1:A:308:GLU:HG3	1.79	0.82
1:A:84:GLY:HA2	1:A:90:LYS:HG2	1.64	0.80
1:A:308:GLU:HB2	3:A:461:HOH:O	1.83	0.79
1:A:258:MET:SD	1:A:283:GLU:HG2	2.22	0.79
1:A:306:PHE:O	1:A:310:GLU:HG3	1.84	0.78
1:A:153:THR:CG2	1:A:158:GLN:HB2	2.14	0.74
1:A:148:ASN:ND2	3:A:522:HOH:O	2.20	0.73
1:A:12:PHE:HB3	1:A:15:LEU:HD21	1.71	0.73
1:A:2:ILE:CG2	1:A:91:PRO:HB3	2.20	0.72
1:A:27:ASP:HB3	3:A:517:HOH:O	1.90	0.71
1:A:58:THR:HG22	1:A:206:TYR:CD1	2.26	0.70
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.56	0.70
1:A:292:GLN:H	1:A:292:GLN:NE2	1.85	0.69
1:A:288:GLY:O	3:A:522:HOH:O	2.12	0.68
1:A:292:GLN:HE21	1:A:292:GLN:N	1.86	0.67
1:A:58:THR:HG22	1:A:206:TYR:CE1	2.31	0.65
1:A:66:MET:HG2	1:A:299:ALA:HB2	1.79	0.64
1:A:262:LEU:HD12	1:A:262:LEU:N	2.12	0.64
1:A:5:ILE:HD12	1:A:215:TYR:CE2	2.32	0.64
1:A:12:PHE:HB3	1:A:15:LEU:CD2	2.29	0.62
1:A:36:ALA:HA	1:A:88:SER:HB3	1.82	0.62
1:A:103:ARG:HD3	3:A:405:HOH:O	2.01	0.60
1:A:152:MET:HA	1:A:152:MET:HE2	1.84	0.60
1:A:50:PHE:CE2	1:A:119:THR:HG21	2.38	0.59
1:A:25:LEU:HB2	3:A:518:HOH:O	2.02	0.58
1:A:12:PHE:O	1:A:15:LEU:HD22	2.04	0.57
1:A:51:LEU:CD2	1:A:110:ILE:HD11	2.34	0.57
1:A:89:ASP:C	1:A:90:LYS:HG3	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLN:O	1:A:301:GLU:HG2	2.06	0.55
1:A:124:ASP:OD1	1:A:125:TRP:N	2.39	0.55
1:A:309:THR:O	1:A:309:THR:HG22	2.07	0.54
1:A:67:ILE:HG22	1:A:68:PRO:N	2.21	0.54
1:A:112:ARG:HG3	1:A:112:ARG:NH1	2.19	0.53
1:A:142:LYS:HG2	1:A:143:ARG:HG3	1.91	0.53
1:A:248:TRP:CZ2	1:A:250:GLY:HA3	2.44	0.53
1:A:133:LEU:CB	1:A:134:PRO:HD3	2.36	0.53
1:A:258:MET:CE	1:A:283:GLU:HG2	2.38	0.53
1:A:112:ARG:NH1	1:A:112:ARG:CG	2.71	0.53
1:A:129:LEU:O	1:A:132:THR:OG1	2.25	0.53
1:A:269:TYR:N	1:A:270:PRO:HD2	2.25	0.52
1:A:36:ALA:HB3	3:A:518:HOH:O	2.10	0.52
1:A:84:GLY:CA	1:A:90:LYS:HG2	2.38	0.52
1:A:20:PHE:HB3	1:A:39:LEU:HD22	1.93	0.51
1:A:133:LEU:HB2	1:A:134:PRO:CD	2.38	0.51
1:A:2:ILE:HG23	1:A:91:PRO:HB3	1.93	0.51
1:A:142:LYS:CG	1:A:143:ARG:HG3	2.41	0.50
1:A:30:GLY:C	1:A:32:PRO:HD3	2.37	0.49
1:A:39:LEU:HB2	1:A:79:ALA:HB3	1.95	0.49
1:A:123:GLN:HE21	1:A:123:GLN:C	2.21	0.49
1:A:221:LYS:O	1:A:225:MET:HG3	2.13	0.49
1:A:5:ILE:HD12	1:A:215:TYR:CD2	2.48	0.49
1:A:271:MET:O	1:A:272:LYS:C	2.56	0.48
1:A:43:ASN:C	1:A:45:ASP:H	2.22	0.48
1:A:64:ARG:HH11	1:A:64:ARG:HG2	1.78	0.48
1:A:153:THR:HG22	3:A:425:HOH:O	2.12	0.48
1:A:11:ARG:NH2	1:A:207:ALA:O	2.47	0.48
1:A:183:SER:O	1:A:213:THR:HG21	2.14	0.48
1:A:2:ILE:N	1:A:2:ILE:HD13	2.29	0.47
1:A:206:TYR:OH	1:A:293:GLU:OE2	2.28	0.47
1:A:262:LEU:HD12	1:A:262:LEU:H	1.79	0.47
1:A:175:TRP:NE1	2:A:600:DCE:C1	2.78	0.47
1:A:175:TRP:HE1	2:A:600:DCE:C1	2.28	0.46
1:A:269:TYR:N	1:A:270:PRO:CD	2.79	0.46
1:A:153:THR:HG21	1:A:158:GLN:CB	2.24	0.46
1:A:220:ARG:HD3	3:A:434:HOH:O	2.15	0.46
1:A:120:LEU:HD21	1:A:130:GLY:O	2.15	0.46
1:A:213:THR:HA	1:A:216:GLN:OE1	2.16	0.45
1:A:123:GLN:C	1:A:123:GLN:NE2	2.74	0.45
1:A:269:TYR:CB	1:A:270:PRO:HD3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:THR:HG22	1:A:253:PHE:N	2.31	0.45
1:A:30:GLY:C	1:A:32:PRO:CD	2.90	0.45
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.69	0.45
1:A:258:MET:HE2	1:A:283:GLU:CD	2.42	0.45
1:A:296:GLU:O	1:A:300:ARG:HG3	2.16	0.45
1:A:31:TYR:N	1:A:32:PRO:HD3	2.30	0.45
1:A:103:ARG:HD3	1:A:103:ARG:HH11	1.50	0.44
1:A:20:PHE:CB	1:A:39:LEU:HD22	2.47	0.44
1:A:243:PHE:CD1	1:A:243:PHE:C	2.96	0.44
1:A:64:ARG:HG2	1:A:64:ARG:NH1	2.31	0.43
1:A:226:VAL:HG21	2:A:600:DCE:C2	2.47	0.43
1:A:151:LEU:HD12	1:A:271:MET:HE1	2.01	0.43
1:A:94:GLU:HB3	1:A:221:LYS:HB2	2.01	0.43
1:A:259:LYS:HB2	1:A:287:ALA:O	2.19	0.42
1:A:154:ASP:OD1	1:A:157:THR:HG23	2.19	0.42
1:A:36:ALA:CB	3:A:518:HOH:O	2.67	0.42
1:A:31:TYR:N	1:A:32:PRO:CD	2.83	0.42
1:A:6:ARG:HD3	1:A:35:ARG:NH2	2.35	0.41
1:A:28:LEU:HD11	3:A:518:HOH:O	2.20	0.41
1:A:117:ASN:O	3:A:421:HOH:O	2.21	0.41
1:A:210:PHE:HA	1:A:211:PRO:HD2	1.54	0.41
1:A:61:TYR:CE1	1:A:64:ARG:HD3	2.55	0.41
1:A:17:GLN:HE21	1:A:17:GLN:HB3	1.75	0.41
1:A:28:LEU:CD1	3:A:518:HOH:O	2.68	0.41
1:A:154:ASP:CG	1:A:157:THR:HG23	2.45	0.41
1:A:190:PHE:CD1	1:A:190:PHE:C	2.99	0.41
1:A:133:LEU:CB	1:A:134:PRO:CD	2.98	0.41
1:A:154:ASP:OD2	1:A:157:THR:CG2	2.69	0.41
1:A:262:LEU:N	1:A:262:LEU:CD1	2.84	0.40
1:A:269:TYR:CB	1:A:270:PRO:CD	2.99	0.40
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.85	0.40
1:A:162:SER:O	1:A:165:VAL:HG23	2.20	0.40
1:A:146:ILE:HG23	1:A:254:MET:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/310 (99%)	273 (89%)	31 (10%)	4 (1%)	9	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	148	ASN
1	A	44	SER
1	A	156	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/262 (100%)	233 (89%)	29 (11%)	6	7

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ILE
1	A	8	PRO
1	A	9	ASP
1	A	13	SER
1	A	15	LEU
1	A	17	GLN

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Mol	Chain	Res	Type
1	A	27	ASP
1	A	44	SER
1	A	67	ILE
1	A	73	SER
1	A	87	LYS
1	A	88	SER
1	A	112	ARG
1	A	117	ASN
1	A	123	GLN
1	A	142	LYS
1	A	147	MET
1	A	153	THR
1	A	157	THR
1	A	162	SER
1	A	180	VAL
1	A	192	LYS
1	A	197	THR
1	A	210	PHE
1	A	222	PHE
1	A	258	MET
1	A	292	GLN
1	A	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	17	GLN
1	A	104	ASN
1	A	123	GLN
1	A	292	GLN
1	A	297	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DCE	A	600	-	3,3,3	0.48	0	2,2,2	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DCE	A	600	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	DCE	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.